Connecting via Winsock to STN

Welcome to STN International! Enter x:x

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	JAN 11	CA/CAPLUS - Expanded patent coverage to include Russia (Federal Institute of Industrial Property)

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:23:39 ON 24 JAN 2005

=>
=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY     SESSION
FULL ESTIMATED COST                                         8.19        8.19

FILE 'REGISTRY' ENTERED AT 09:46:46 ON 24 JAN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   23 JAN 2005  HIGHEST RN 819046-01-0
DICTIONARY FILE UPDATES:  23 JAN 2005  HIGHEST RN 819046-01-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\aw1.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=>
Uploading C:\STNEXP4\QUERIES\aw2.str

L2      STRUCTURE UPLOADED

=>
Uploading C:\STNEXP4\QUERIES\aw3.str

L3      STRUCTURE UPLOADED


Page 2
```

```
=> s l1
SAMPLE SEARCH INITIATED 09:50:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  61448 TO ITERATE

  1.6% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L4            0 SEA SSS SAM L1

=>
=>
Uploading C:\STNEXP4\QUERIES\aw4.str

L5      STRUCTURE UPLOADED

=> s l5
SAMPLE SEARCH INITIATED 10:09:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  34843 TO ITERATE

  2.9% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      685710 TO   708010
PROJECTED ANSWERS:              0 TO        0

L6            0 SEA SSS SAM L5

=>
Uploading C:\STNEXP4\QUERIES\aw5.str

L7      STRUCTURE UPLOADED

=> s l7
SAMPLE SEARCH INITIATED 10:13:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  49340 TO ITERATE

  2.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      973556 TO  1000044
PROJECTED ANSWERS:              0 TO        0

L8            0 SEA SSS SAM L7

=>
Uploading C:\STNEXP4\QUERIES\aw6.str
```

```
L9      STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 10:18:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  46756 TO ITERATE

  2.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       922223 TO   948017
PROJECTED ANSWERS:               0 TO        0

L10           0 SEA SSS SAM L9

=>

=>
Uploading C:\STNEXP4\QUERIES\aw7.str

L11     STRUCTURE UPLOADED

=> s l11
SAMPLE SEARCH INITIATED 10:20:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   4837 TO ITERATE

 20.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        92570 TO   100910
PROJECTED ANSWERS:               0 TO        0

L12           0 SEA SSS SAM L11

=>
Uploading C:\STNEXP4\QUERIES\aw8.str

L13     STRUCTURE UPLOADED

=> s l13
SAMPLE SEARCH INITIATED 10:21:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  10214 TO ITERATE

  9.8% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       198224 TO   210336
PROJECTED ANSWERS:               0 TO        0

L14           0 SEA SSS SAM L13
```

```
=> search l11
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:21:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  96489 TO ITERATE

100.0% PROCESSED   96489 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.14

L15           0 SEA SSS FUL L11

=> search l13
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:22:07 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED  203759 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.13

L16           0 SEA SSS FUL L13

=>
Uploading C:\STNEXP4\QUERIES\aw10.str

L17     STRUCTURE UPLOADED

=>
Uploading C:\STNEXP4\QUERIES\aw9.str

L18     STRUCTURE UPLOADED

=> s l17
SAMPLE SEARCH INITIATED 10:25:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   4837 TO ITERATE

 20.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        92570 TO   100910
PROJECTED ANSWERS:               0 TO        0

L19           0 SEA SSS SAM L17

=> search l17
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:25:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  96489 TO ITERATE

100.0% PROCESSED   96489 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.15

L20           0 SEA SSS FUL L17
```

```
=> s l18
SAMPLE SEARCH INITIATED 10:26:01 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  10214 TO ITERATE

  9.8% PROCESSED    1000 ITERATIONS                          0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       198224 TO   210336
PROJECTED ANSWERS:               0 TO        0

L21           0 SEA SSS SAM L18

=> search l18
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:26:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 203759 TO ITERATE

100.0% PROCESSED  203759 ITERATIONS                      21 ANSWERS
SEARCH TIME: 00.00.14

L22          21 SEA SSS FUL L18

=>
Uploading C:\STNEXP4\QUERIES\all.str

L23     STRUCTURE UPLOADED

=> d l23
L23 HAS NO ANSWERS
L23             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l23
SAMPLE SEARCH INITIATED 10:32:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    177 TO ITERATE

100.0% PROCESSED     177 ITERATIONS  (    19 INCOMPLETE)      19 ANSWERS
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2742 TO     4338
PROJECTED ANSWERS:             119 TO      641

L24          19 SEA SSS SAM L23

=> s l23
SAMPLE SEARCH INITIATED 10:32:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    177 TO ITERATE

100.0% PROCESSED     177 ITERATIONS  (    19 INCOMPLETE)      19 ANSWERS
```

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2742 TO 4338
PROJECTED ANSWERS: 119 TO 641

L25 19 SEA SSS SAM L23

=> search l23
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 10:33:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3334 TO ITERATE

100.0% PROCESSED 3334 ITERATIONS (300 INCOMPLETE) 300 ANSWERS
SEARCH TIME: 00.00.11

L26 300 SEA SSS FUL L23

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	838.04	846.23

FILE 'CAPLUS' ENTERED AT 10:33:22 ON 24 JAN 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 24 Jan 2005 VOL 142 ISS 5
FILE LAST UPDATED: 23 Jan 2005 (20050123/ED)

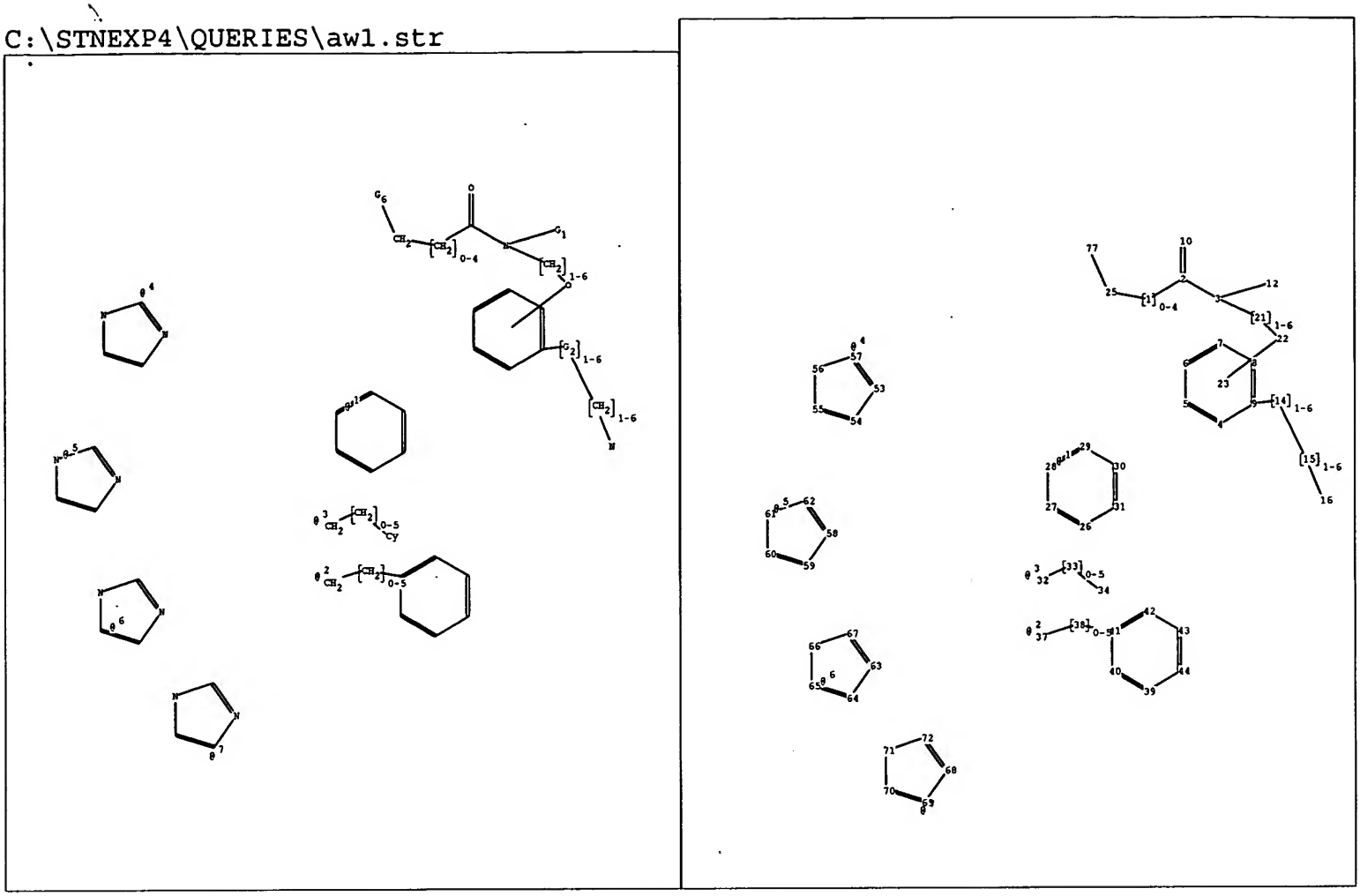
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l26
L27 123 L26

=> d l27 fbib ab hitstr 1-123

L27 ANSWER 1 OF 123 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:1059377 CAPLUS
DN 142:19573
TI Purification means
IN Hay, Alastair; Cotton, Graham; Ramage, Robert
PA CSS-Albachem Limited, UK

C:\STNEXP4\QUERIES\aw1.str



chain nodes :
1 2 3 10 12 14 15 16 21 22 25 32 33 34 37 38 77
ring nodes :
4 5 6 7 8 9 26 27 28 29 30 31 39 40 41 42 43 44 53 54
55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
chain bonds :
1-2 1-25 2-3 2-10 3-12 3-21 9-14 14-15 15-16 21-22 25-77 32-33
33-34 37-38 38-41
ring bonds :
4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 27-28 28-29 29-30 30-31
39-40 39-44 40-41 41-42 42-43 43-44 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62 63-64 63-67 64-65 65-66
66-67 68-69 68-72 69-70 70-71 71-72
exact/norm bonds :
2-3 2-10 3-12 9-14 14-15 25-77 33-34 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62 63-64 63-67 64-65 65-66
66-67 68-69 68-72 69-70 70-71 71-72
exact bonds :
1-2 1-25 3-21 15-16 21-22 32-33 37-38 38-41
normalized bonds :
4-5 4-9 5-6 6-7 7-8 8-9 26-27 26-31 27-28 28-29 29-30 30-31
39-40 39-44 40-41 41-42 42-43 43-44

G1:H,Ak

G2:O,N,C

G3:O,CH2

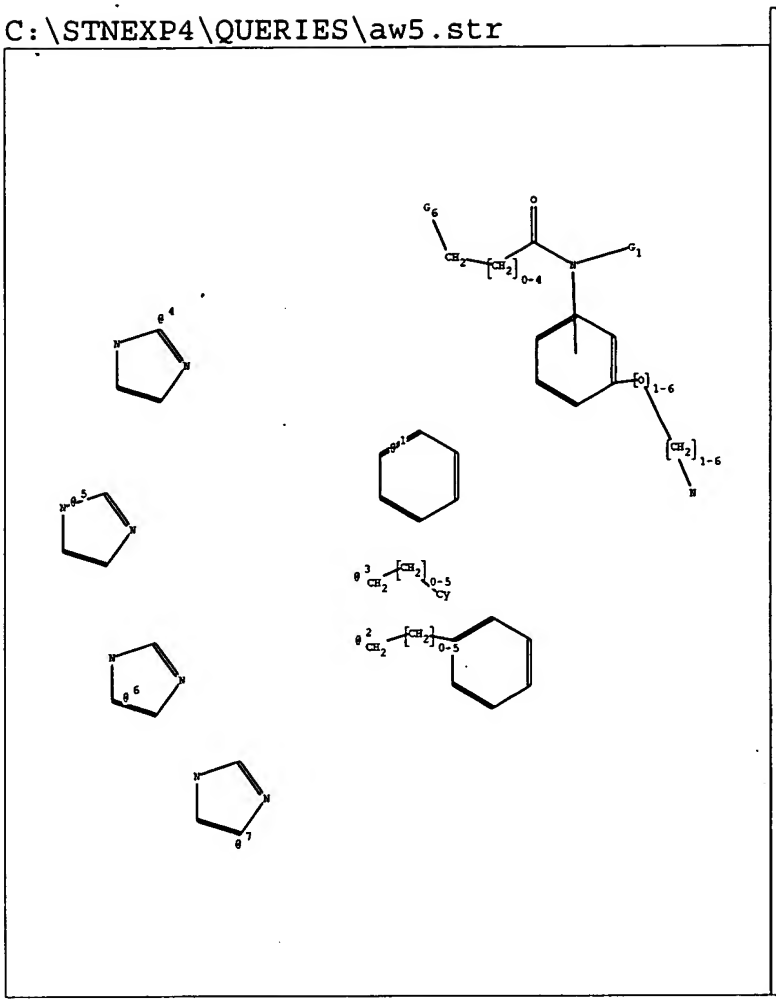
G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

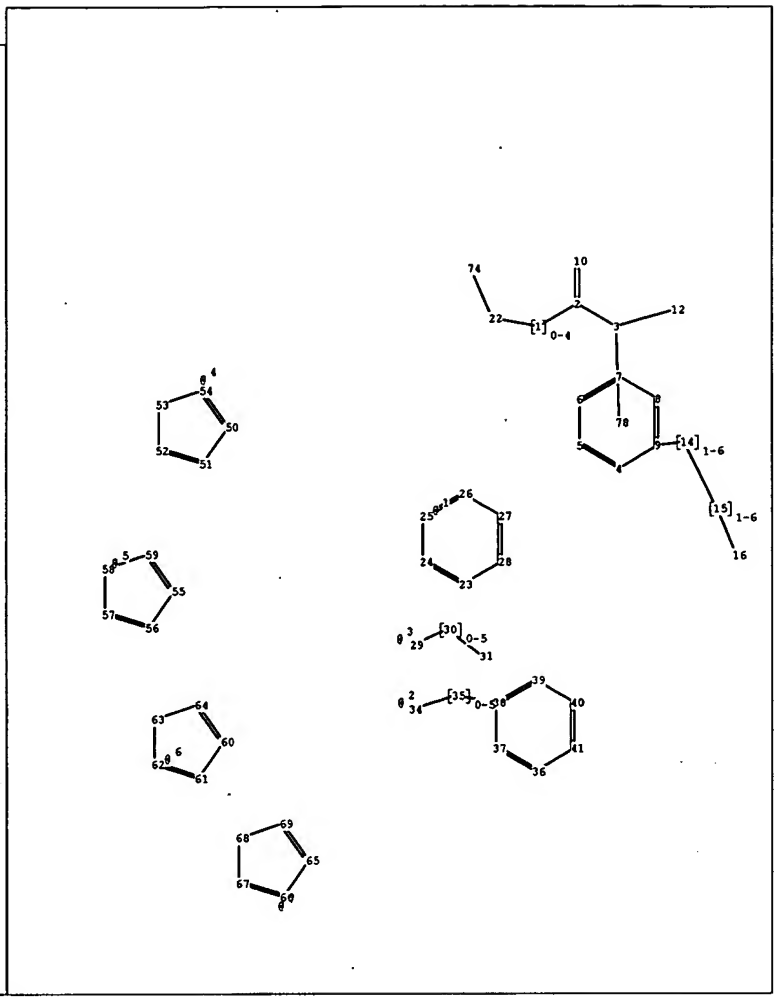
G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 21:CLASS 22:CLASS
23:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:CLASS 33:CLASS 34:Atom 37:CLASS 38:CLASS 39:Atom 40:Atom
41:Atom 42:Atom 43:Atom 44:Atom 53:Atom 54:Atom 55:Atom 56:Atom
57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom
65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom
77:CLASS

C:\STNEXP4\QUERIES\aw5.str





chain nodes :
1 2 3 10 12 14 15 16 22 29 30 31 34 35 74
ring nodes :
4 5 6 7 8 9 23 24 25 26 27 28 36 37 38 39 40 41 50 51
52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69
chain bonds :
1-2 1-22 2-3 2-10 3-12 9-14 14-15 15-16 22-74 29-30 30-31
34-35 35-38
ring bonds :
4-5 4-9 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28
36-37 36-41 37-38 38-39 39-40 40-41 50-51 50-54 51-52 52-53
53-54 55-56 55-59 56-57 57-58 58-59 60-61 60-64 61-62 62-63
63-64 65-66 65-69 66-67 67-68 68-69
exact/norm bonds :
2-3 2-10 3-12 9-14 22-74 30-31 50-51 50-54 51-52 52-53 53-54
55-56 55-59 56-57 57-58 58-59 60-61 60-64 61-62 62-63 63-64
65-66 65-69 66-67 67-68 68-69
exact bonds :
1-2 1-22 14-15 15-16 29-30 34-35 35-38
normalized bonds :
4-5 4-9 5-6 6-7 7-8 8-9 23-24 23-28 24-25 25-26 26-27 27-28
36-37 36-41 37-38 38-39 39-40 40-41

G1:H,Ak

G2:O,N,C

G3:O,CH2

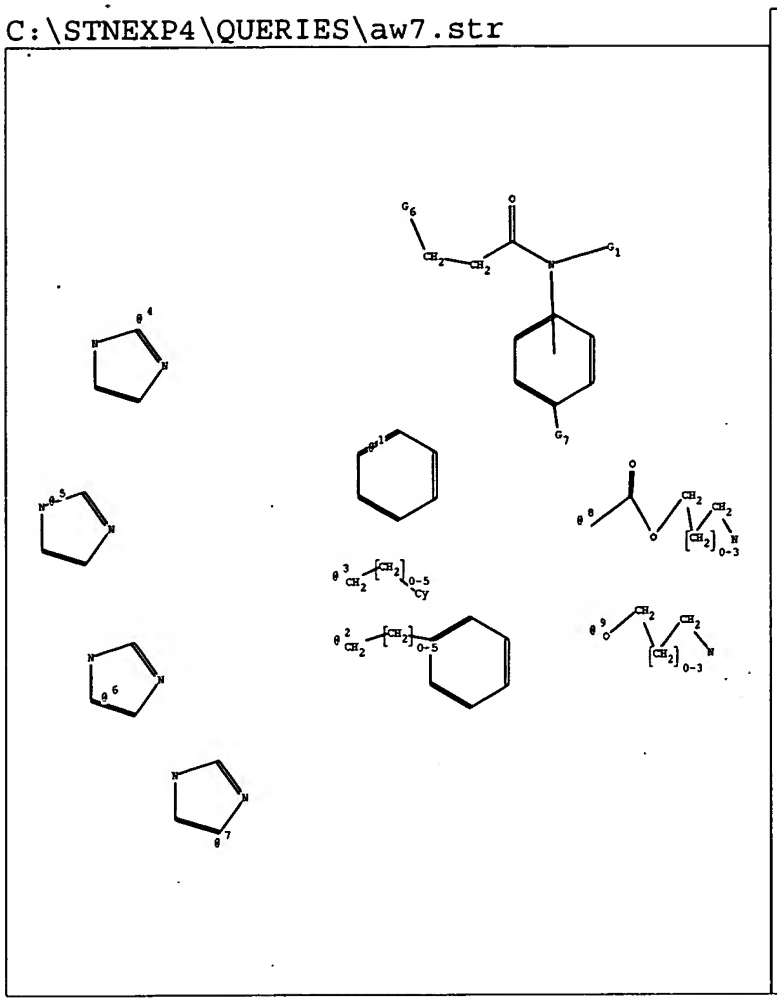
G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

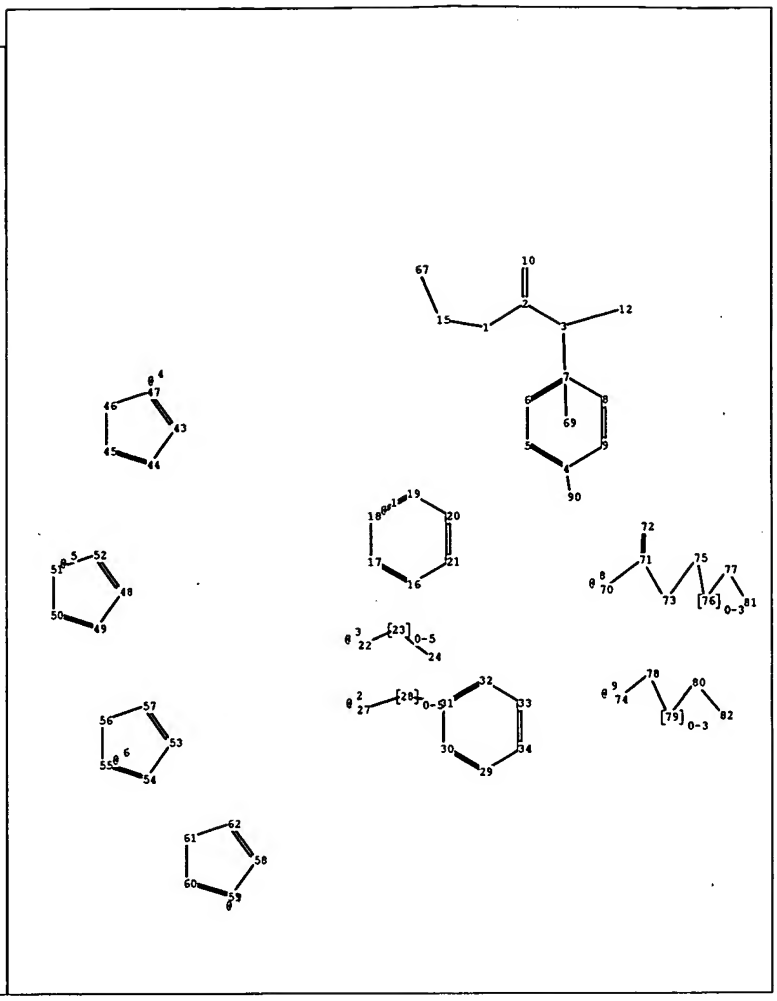
G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 22:CLASS 23:Atom
24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS 31:Atom
34:CLASS 35:CLASS 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom
58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom
66:Atom 67:Atom 68:Atom 69:Atom 74:CLASS 78:CLASS

C:\STNEXP4\QUERIES\aw7.str





chain nodes :
1 2 3 10 12 15 22 23 24 27 28 67 70 71 72 73 74 75 76
77 78 79 80 81 82 90
ring nodes :
4 5 6 7 8 9 16 17 18 19 20 21 29 30 31 32 33 34 43 44
45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62
chain bonds :
1-2 1-15 2-3 2-10 3-12 4-90 15-67 22-23 23-24 27-28 28-31
70-71 71-72 71-73 73-75 74-78 75-76 76-77 77-81 78-79 79-80
80-82
ring bonds :
4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21
29-30 29-34 30-31 31-32 32-33 33-34 43-44 43-47 44-45 45-46
46-47 48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56
56-57 58-59 58-62 59-60 60-61 61-62
exact/norm bonds :
2-3 2-10 3-12 4-90 15-67 23-24 43-44 43-47 44-45 45-46 46-47
48-49 48-52 49-50 50-51 51-52 53-54 53-57 54-55 55-56 56-57
58-59 58-62 59-60 60-61 61-62 71-72 71-73
exact bonds :
1-2 1-15 22-23 27-28 28-31 70-71 73-75 74-78 75-76 76-77 77-81
78-79 79-80 80-82
normalized bonds :
4-5 4-9 5-6 6-7 7-8 8-9 16-17 16-21 17-18 18-19 19-20 20-21
29-30 29-34 30-31 31-32 32-33 33-34

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

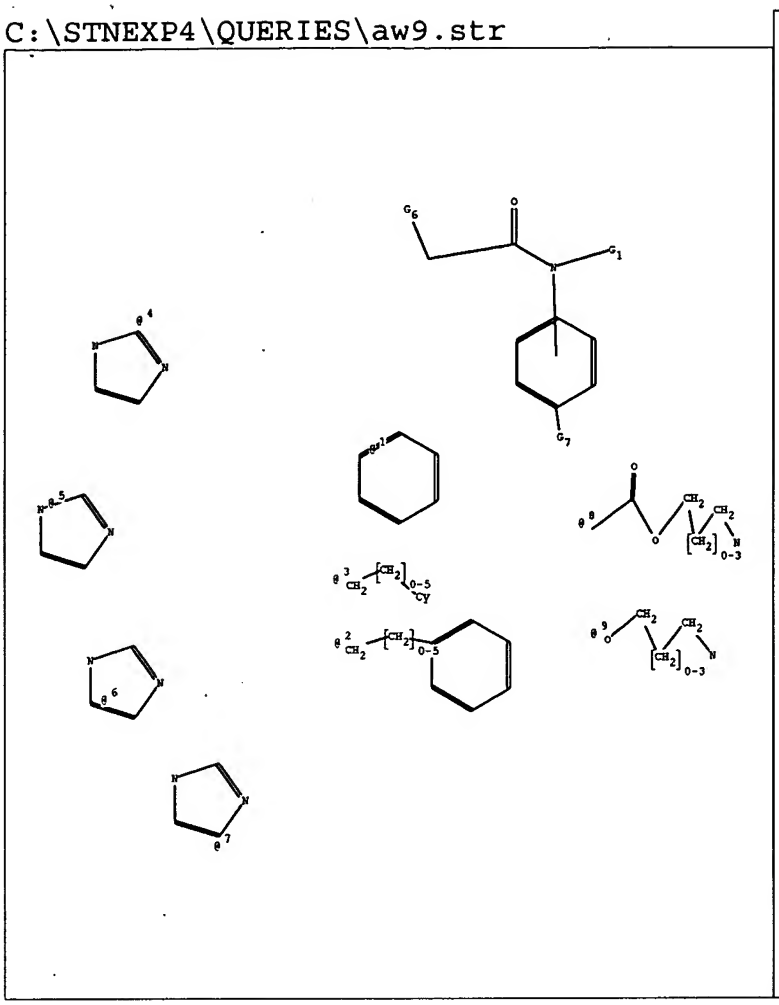
G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

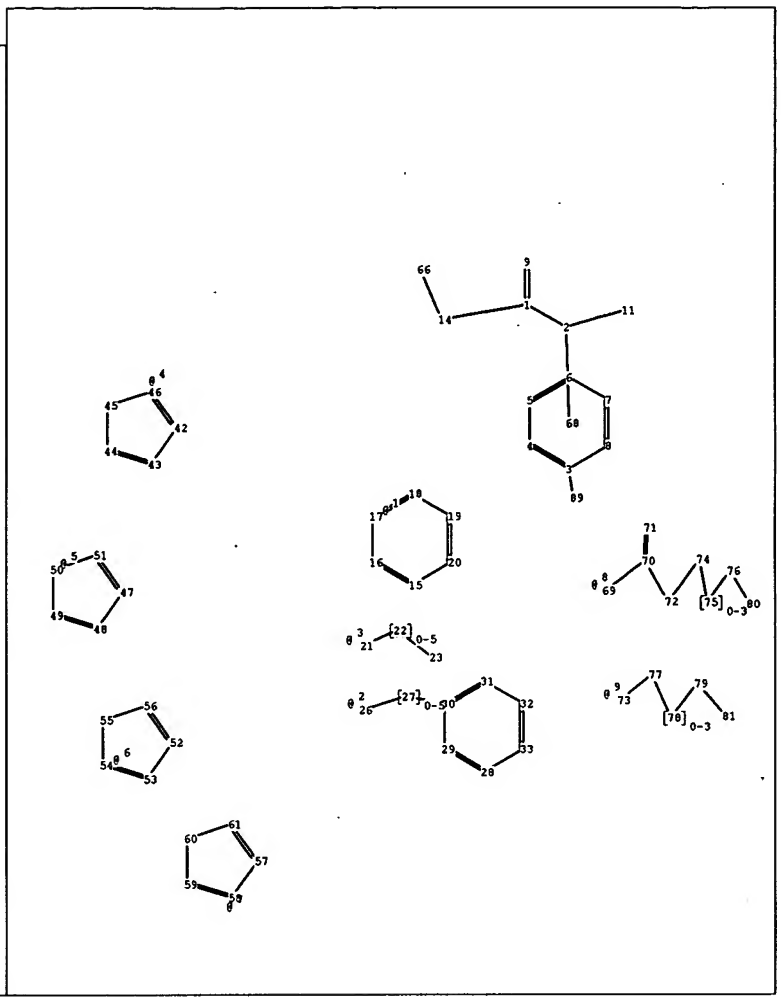
G7:[*8],[*9]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:CLASS 12:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:CLASS 23:CLASS 24:Atom 27:CLASS 28:CLASS 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
62:Atom 67:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
81:CLASS 82:CLASS 90:CLASS

C:\STNEXP4\QUERIES\aw9.str





chain nodes :
1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89
ring nodes :
3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61
chain bonds :
1-9 1-2 1-14 2-11 3-89 14-66 21-22 22-23 26-27 27-30 69-70
70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72
exact bonds :
1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80
77-78 78-79 79-81
normalized bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS
11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:Atom 26:CLASS 27:CLASS 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
66:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
81:CLASS 89:CLASS

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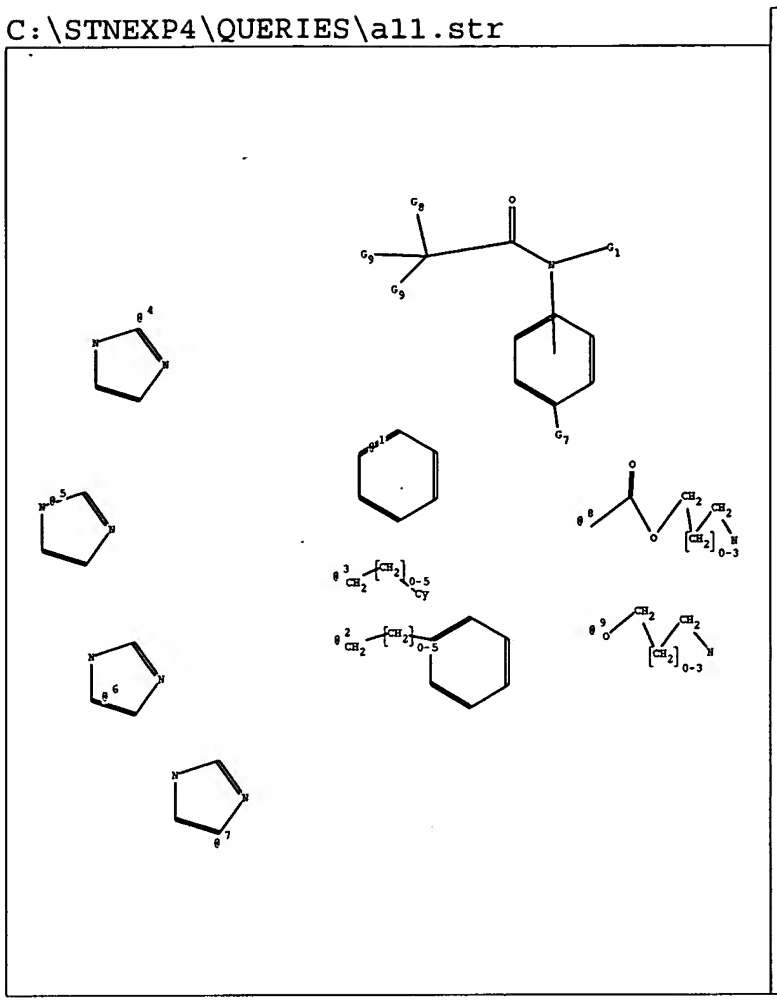

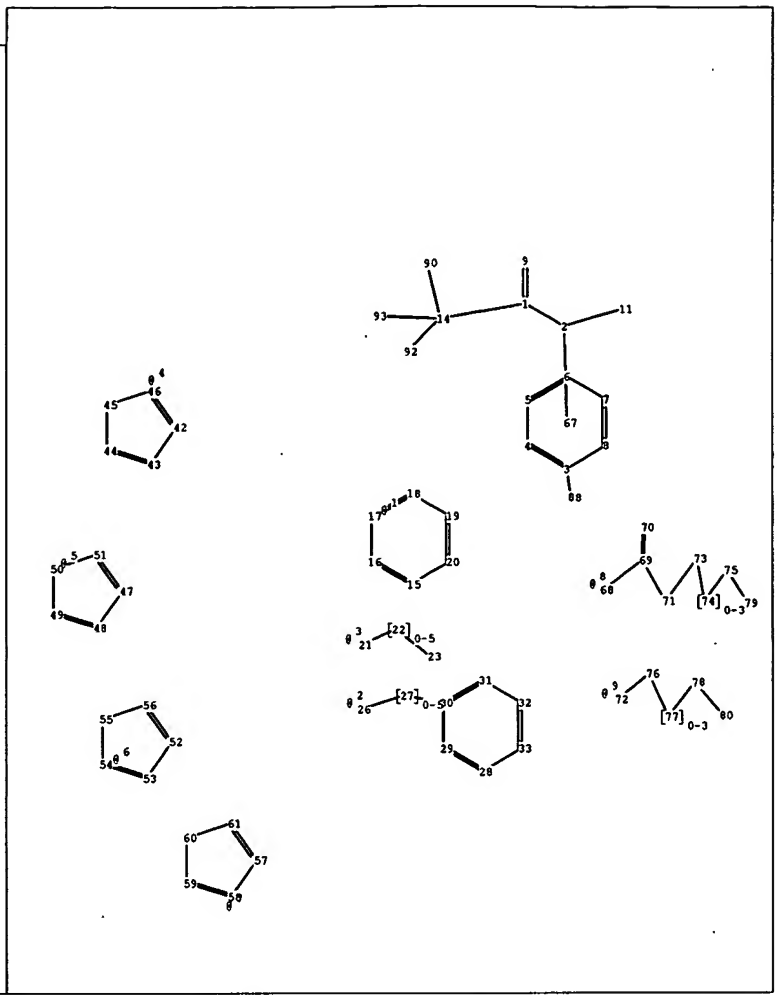

chain nodes :
1 2 9 11 14 21 22 23 26 27 68 69 70 71 72 73 74 75 76
77 78 79 80 88 90 92 93
ring nodes :
3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61
chain bonds :
1-9 1-2 1-14 2-11 3-88 14-90 14-92 14-93 21-22 22-23 26-27
27-30 68-69 69-70 69-71 71-73 72-76 73-74 74-75 75-79 76-77
77-78 78-80
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-9 1-2 2-11 3-88 14-90 14-92 14-93 22-23 42-43 42-46 43-44
44-45 45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54
54-55 55-56 57-58 57-61 58-59 59-60 60-61 69-70 69-71
exact bonds :
1-14 21-22 26-27 27-30 68-69 71-73 72-76 73-74 74-75 75-79
76-77 77-78 78-80
normalized bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

G8:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1]

G9:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1]

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS
11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:Atom 26:CLASS 27:CLASS 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
88:CLASS 90:CLASS 92:CLASS 93:CLASS

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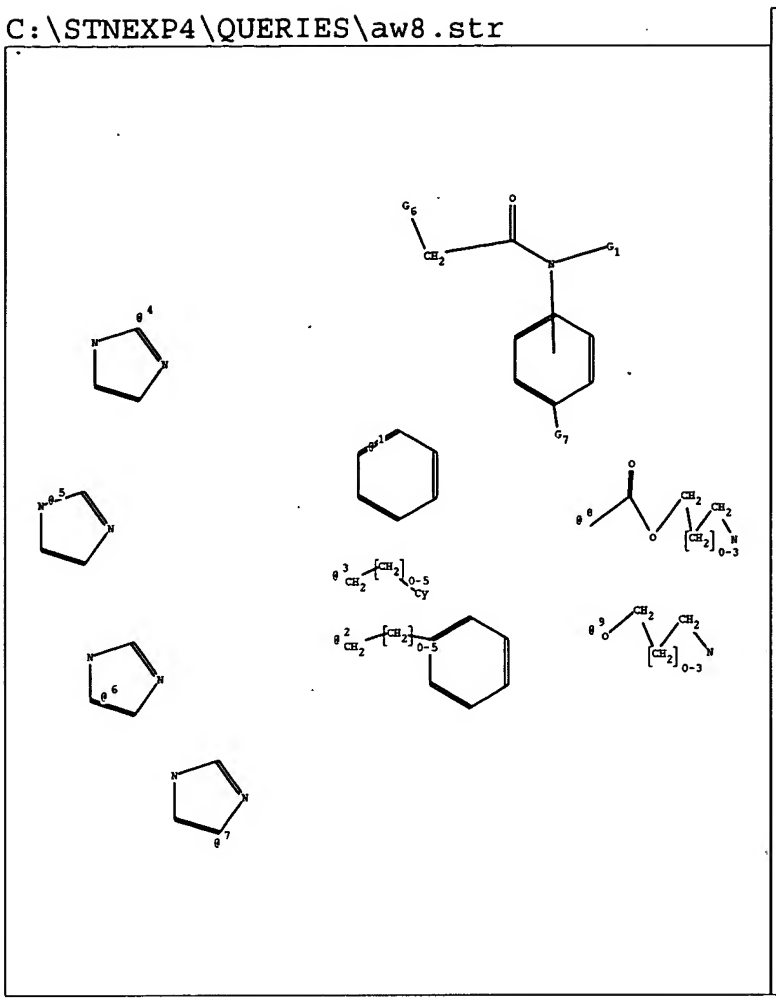

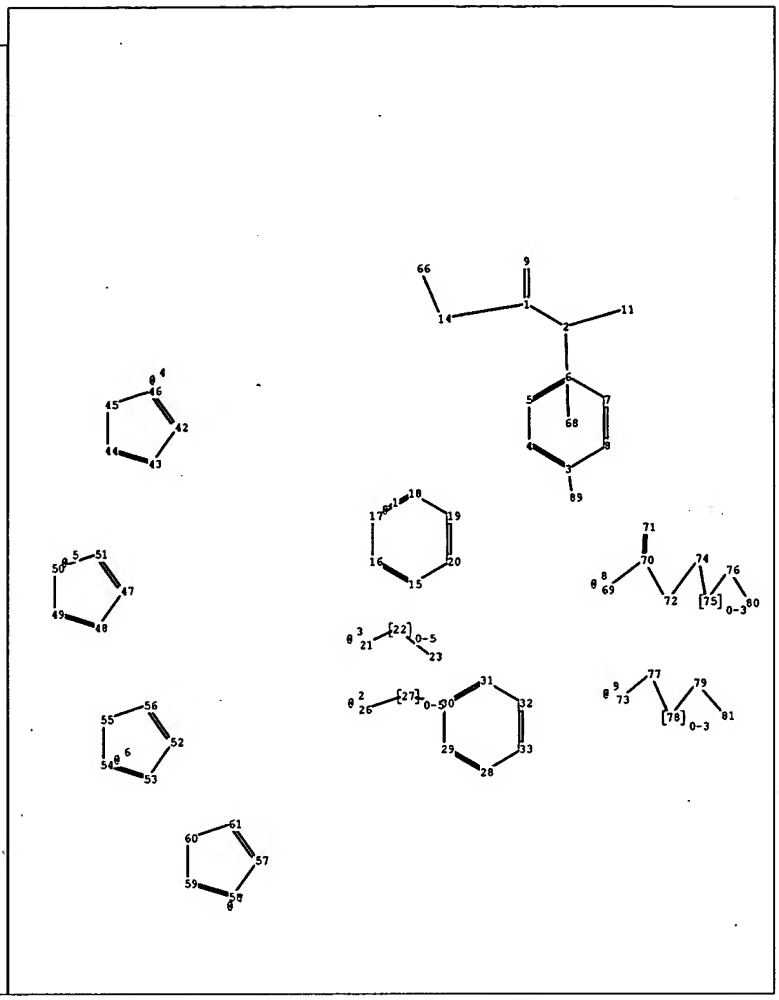

chain nodes :
1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89
ring nodes :
3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61
chain bonds :
1-9 1-2 1-14 2-11 3-89 14-66 21-22 22-23 26-27 27-30 69-70
70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79 79-81
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72
exact bonds :
1-14 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76 76-80
77-78 78-79 79-81
normalized bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS
11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:Atom 26:CLASS 27:CLASS 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom
66:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
81:CLASS 89:CLASS

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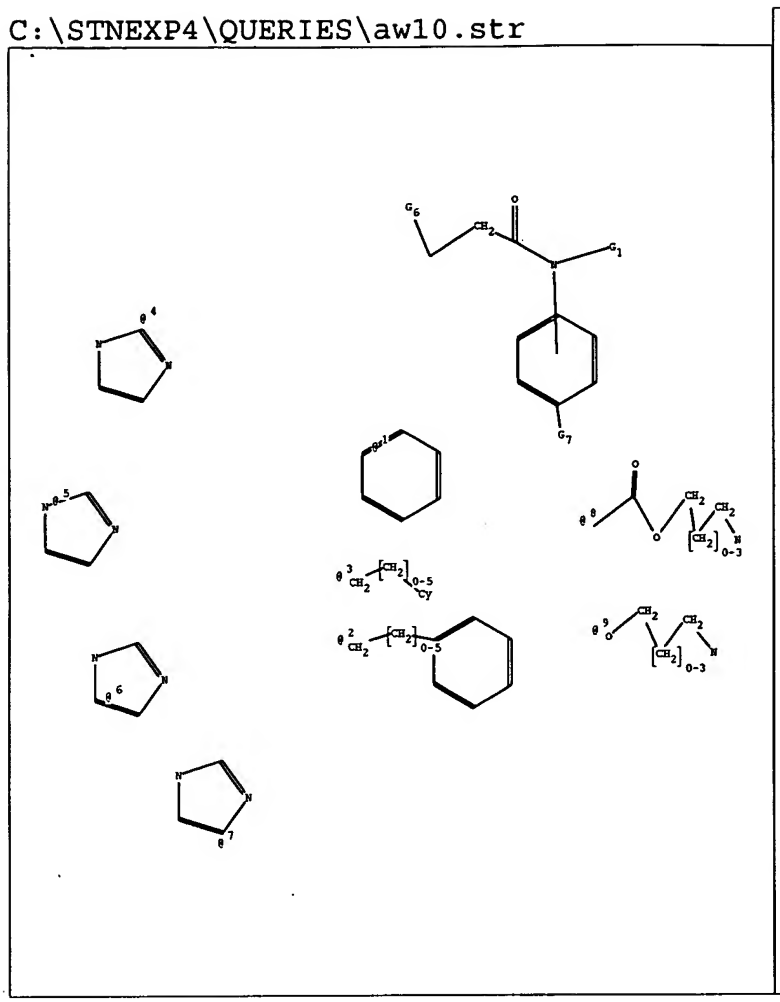

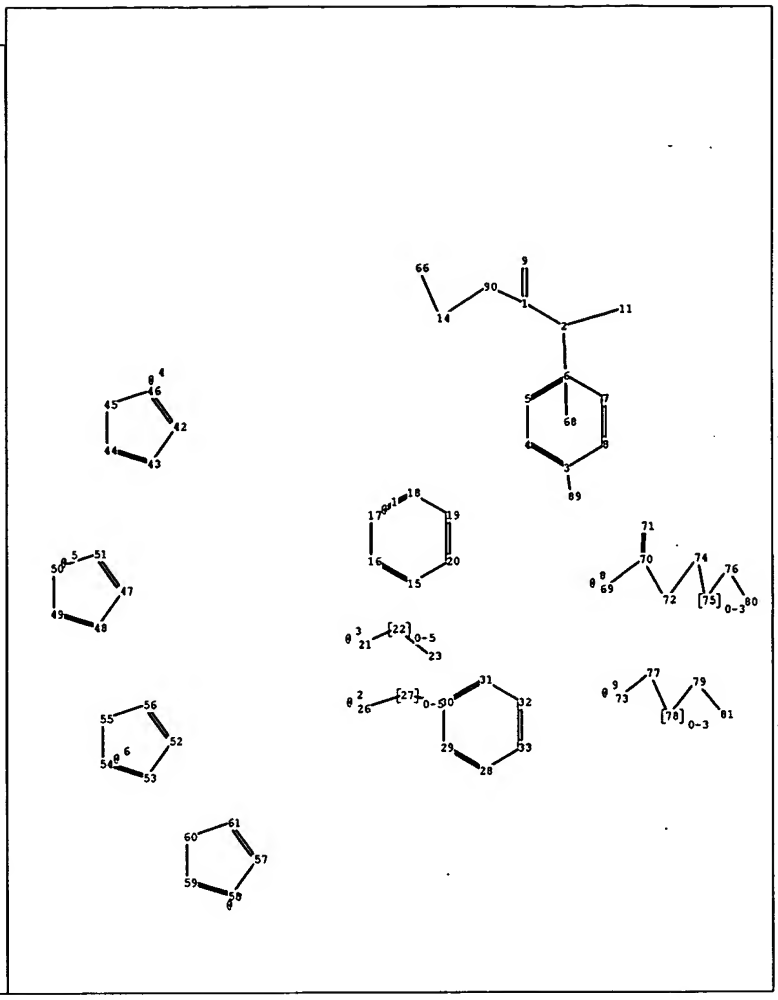

chain nodes :
1 2 9 11 14 21 22 23 26 27 66 69 70 71 72 73 74 75 76
77 78 79 80 81 89 90
ring nodes :
3 4 5 6 7 8 15 16 17 18 19 20 28 29 30 31 32 33 42 43
44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61
chain bonds :
1-9 1-2 1-90 2-11 3-89 14-66 14-90 21-22 22-23 26-27 27-30
69-70 70-71 70-72 72-74 73-77 74-75 75-76 76-80 77-78 78-79
79-81
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33 42-43 42-46 43-44 44-45
45-46 47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55
55-56 57-58 57-61 58-59 59-60 60-61
exact/norm bonds :
1-9 1-2 2-11 3-89 14-66 22-23 42-43 42-46 43-44 44-45 45-46
47-48 47-51 48-49 49-50 50-51 52-53 52-56 53-54 54-55 55-56
57-58 57-61 58-59 59-60 60-61 70-71 70-72
exact bonds :
1-90 14-90 21-22 26-27 27-30 69-70 72-74 73-77 74-75 75-76
76-80 77-78 78-79 79-81
normalized bonds :
3-4 3-8 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

G1:H,Ak

G2:O,N,C

G3:O,CH2

G4:H,CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,[*1],[*2]

G5:CH3,Et,n-Pr,i-Pr,i-Bu,s-Bu,t-Bu,[*1],[*3]

G6:NH2,NH,[*1],[*4],[*5],[*6],[*7]

G7:[*8],[*9]

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS
11:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:Atom 26:CLASS 27:CLASS 28:Atom 29:Atom
30:Atom 31:Atom 32:Atom 33:Atom 42:Atom 43:Atom 44:Atom 45:Atom
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66:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS
74:CLASS 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS 80:CLASS
81:CLASS 89:CLASS 90:CLASS